



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 8, 2024 – 04:07 PM EDT

PDB ID : 8UWB
Title : Crystal structure of PP2A PPP2R1A-PPP2CA-PPP2R5E phosphatase.
Authors : Wachter, F.; Nowak, R.P.; Fischer, E.S.
Deposited on : 2023-11-06
Resolution : 3.15 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.36.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36.1

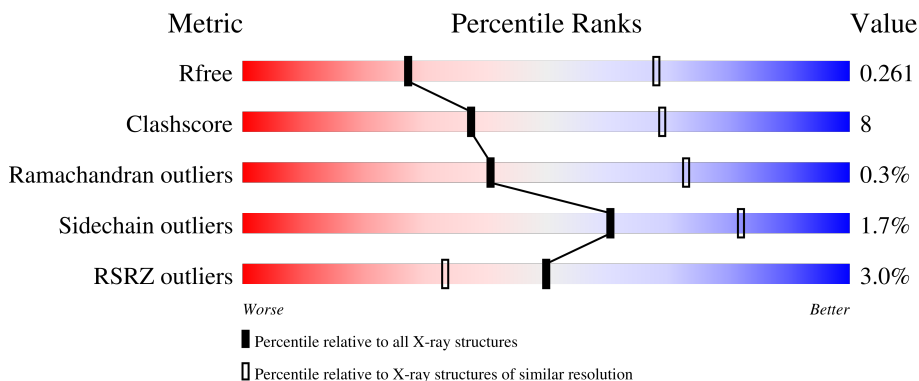
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.15 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.




Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1665 (3.20-3.12)
Clashscore	141614	1804 (3.20-3.12)
Ramachandran outliers	138981	1770 (3.20-3.12)
Sidechain outliers	138945	1769 (3.20-3.12)
RSRZ outliers	127900	1616 (3.20-3.12)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	612	
1	D	612	
2	B	467	
2	E	467	
3	C	333	

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Mol	Chain	Length	Quality of chain
3	F	333	 74% 19% 7%

2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 20861 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Serine/threonine-protein phosphatase 2A catalytic subunit alpha isoform.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	589	Total	C	N	O	S	0	0	0
			4578	2905	771	874	28			
1	D	573	Total	C	N	O	S	0	0	0
			4466	2834	755	850	27			

There are 46 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-22	MET	-	initiating methionine	UNP P30153
A	-21	ASP	-	expression tag	UNP P30153
A	-20	TYR	-	expression tag	UNP P30153
A	-19	LYS	-	expression tag	UNP P30153
A	-18	ASP	-	expression tag	UNP P30153
A	-17	ASP	-	expression tag	UNP P30153
A	-16	ASP	-	expression tag	UNP P30153
A	-15	ASP	-	expression tag	UNP P30153
A	-14	LYS	-	expression tag	UNP P30153
A	-13	SER	-	expression tag	UNP P30153
A	-12	ALA	-	expression tag	UNP P30153
A	-11	VAL	-	expression tag	UNP P30153
A	-10	ASP	-	expression tag	UNP P30153
A	-9	GLU	-	expression tag	UNP P30153
A	-8	ASN	-	expression tag	UNP P30153
A	-7	LEU	-	expression tag	UNP P30153
A	-6	TYR	-	expression tag	UNP P30153
A	-5	PHE	-	expression tag	UNP P30153
A	-4	GLN	-	expression tag	UNP P30153
A	-3	GLY	-	expression tag	UNP P30153
A	-2	GLY	-	expression tag	UNP P30153
A	-1	GLY	-	expression tag	UNP P30153
A	0	ARG	-	expression tag	UNP P30153
D	-22	MET	-	initiating methionine	UNP P30153

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-21	ASP	-	expression tag	UNP P30153
D	-20	TYR	-	expression tag	UNP P30153
D	-19	LYS	-	expression tag	UNP P30153
D	-18	ASP	-	expression tag	UNP P30153
D	-17	ASP	-	expression tag	UNP P30153
D	-16	ASP	-	expression tag	UNP P30153
D	-15	ASP	-	expression tag	UNP P30153
D	-14	LYS	-	expression tag	UNP P30153
D	-13	SER	-	expression tag	UNP P30153
D	-12	ALA	-	expression tag	UNP P30153
D	-11	VAL	-	expression tag	UNP P30153
D	-10	ASP	-	expression tag	UNP P30153
D	-9	GLU	-	expression tag	UNP P30153
D	-8	ASN	-	expression tag	UNP P30153
D	-7	LEU	-	expression tag	UNP P30153
D	-6	TYR	-	expression tag	UNP P30153
D	-5	PHE	-	expression tag	UNP P30153
D	-4	GLN	-	expression tag	UNP P30153
D	-3	GLY	-	expression tag	UNP P30153
D	-2	GLY	-	expression tag	UNP P30153
D	-1	GLY	-	expression tag	UNP P30153
D	0	ARG	-	expression tag	UNP P30153

- Molecule 2 is a protein called Serine/threonine-protein phosphatase 2A 56 kDa regulatory subunit epsilon isoform.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	410	3420	2227	552	624	17	0	1	0
2	E	407	3383	2204	546	616	17	0	0	0

- Molecule 3 is a protein called Serine/threonine-protein phosphatase 2A 65 kDa regulatory subunit A alpha isoform.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	309	2505	1584	432	473	16	0	0	0
3	F	309	2505	1584	432	473	16	0	0	0

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	-23	MET	-	initiating methionine	UNP P67775
F	-22	ASP	-	expression tag	UNP P67775
F	-21	TRP	-	expression tag	UNP P67775
F	-20	SER	-	expression tag	UNP P67775
F	-19	HIS	-	expression tag	UNP P67775
F	-18	PRO	-	expression tag	UNP P67775
F	-17	GLN	-	expression tag	UNP P67775
F	-16	PHE	-	expression tag	UNP P67775
F	-15	GLU	-	expression tag	UNP P67775
F	-14	LYS	-	expression tag	UNP P67775
F	-13	SER	-	expression tag	UNP P67775
F	-12	ALA	-	expression tag	UNP P67775
F	-11	VAL	-	expression tag	UNP P67775
F	-10	ASP	-	expression tag	UNP P67775
F	-9	GLU	-	expression tag	UNP P67775
F	-8	ASN	-	expression tag	UNP P67775
F	-7	LEU	-	expression tag	UNP P67775
F	-6	TYR	-	expression tag	UNP P67775
F	-5	PHE	-	expression tag	UNP P67775
F	-4	GLN	-	expression tag	UNP P67775
F	-3	GLY	-	expression tag	UNP P67775
F	-2	GLY	-	expression tag	UNP P67775
F	-1	GLY	-	expression tag	UNP P67775
F	0	ARG	-	expression tag	UNP P67775
C	-23	MET	-	initiating methionine	UNP P67775
C	-22	ASP	-	expression tag	UNP P67775
C	-21	TRP	-	expression tag	UNP P67775
C	-20	SER	-	expression tag	UNP P67775
C	-19	HIS	-	expression tag	UNP P67775
C	-18	PRO	-	expression tag	UNP P67775
C	-17	GLN	-	expression tag	UNP P67775
C	-16	PHE	-	expression tag	UNP P67775
C	-15	GLU	-	expression tag	UNP P67775
C	-14	LYS	-	expression tag	UNP P67775
C	-13	SER	-	expression tag	UNP P67775
C	-12	ALA	-	expression tag	UNP P67775
C	-11	VAL	-	expression tag	UNP P67775
C	-10	ASP	-	expression tag	UNP P67775
C	-9	GLU	-	expression tag	UNP P67775
C	-8	ASN	-	expression tag	UNP P67775
C	-7	LEU	-	expression tag	UNP P67775
C	-6	TYR	-	expression tag	UNP P67775
C	-5	PHE	-	expression tag	UNP P67775

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-4	GLN	-	expression tag	UNP P67775
C	-3	GLY	-	expression tag	UNP P67775
C	-2	GLY	-	expression tag	UNP P67775
C	-1	GLY	-	expression tag	UNP P67775
C	0	ARG	-	expression tag	UNP P67775

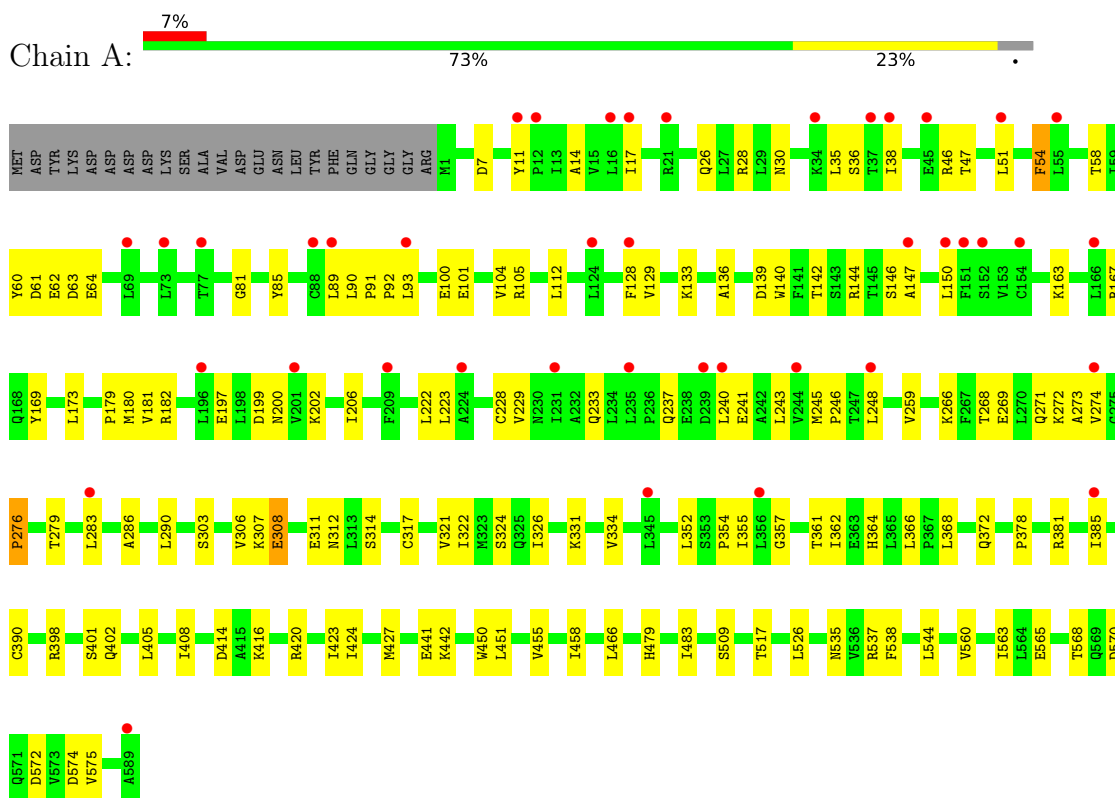
- Molecule 4 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	2	Total	Mn	0	0
			2	2		
4	F	2	Total	Mn	0	0
			2	2		

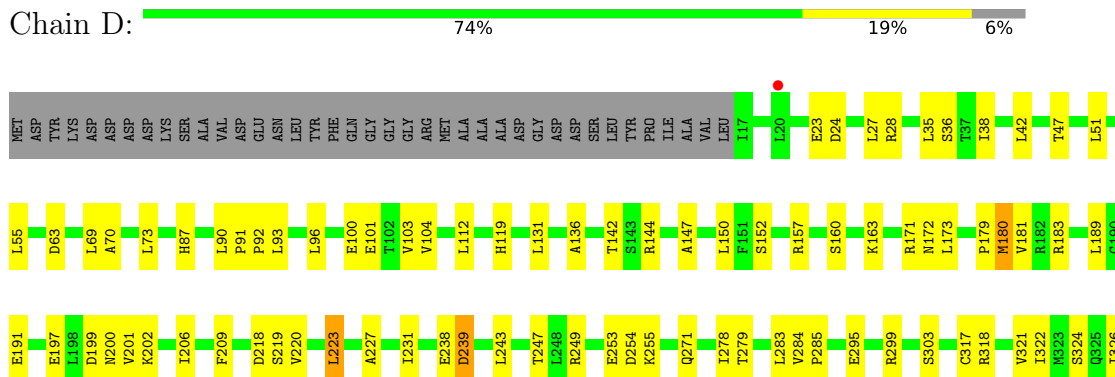
3 Residue-property plots [i](#)

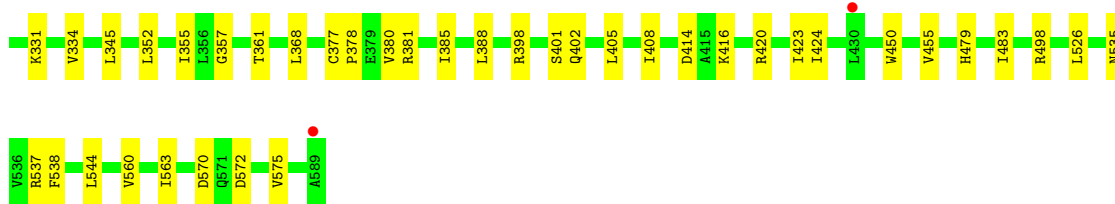
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Serine/threonine-protein phosphatase 2A catalytic subunit alpha isoform

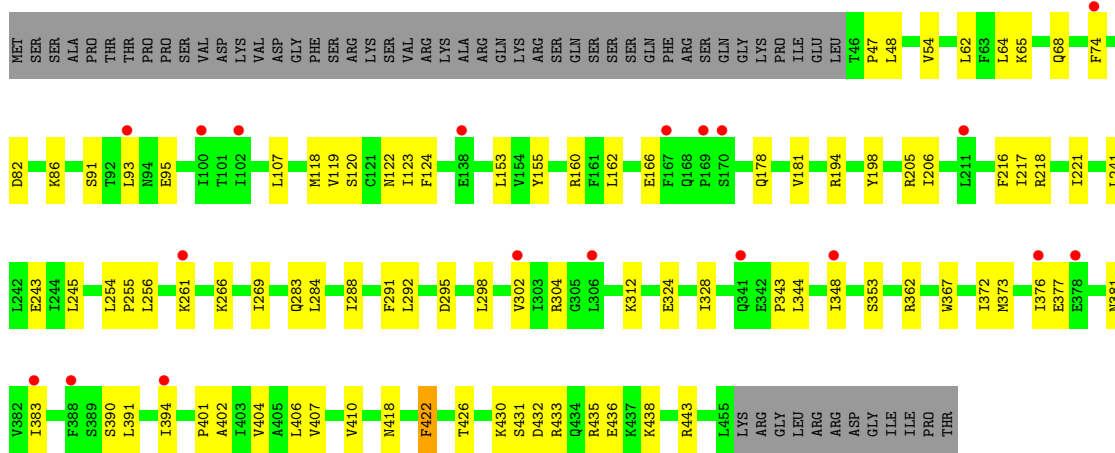


- Molecule 1: Serine/threonine-protein phosphatase 2A catalytic subunit alpha isoform

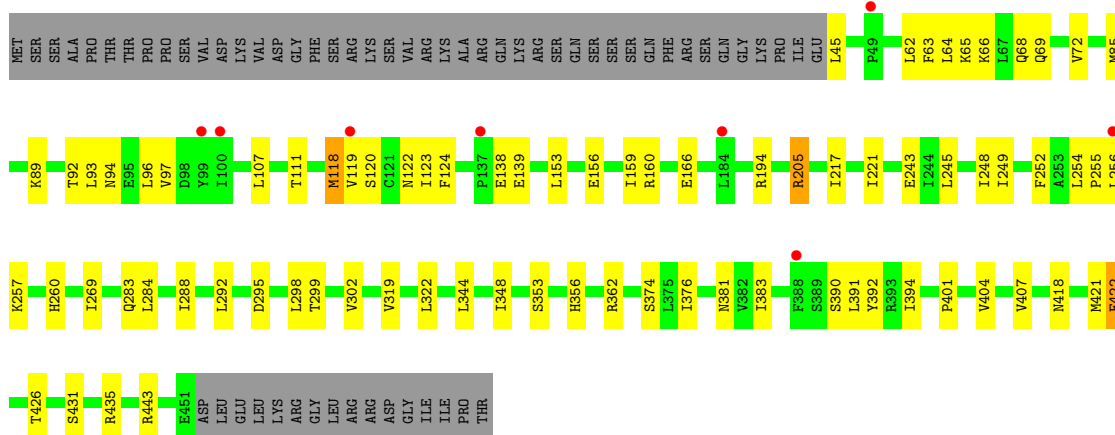




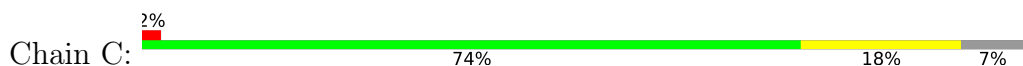
- Molecule 2: Serine/threonine-protein phosphatase 2A 56 kDa regulatory subunit epsilon isoform

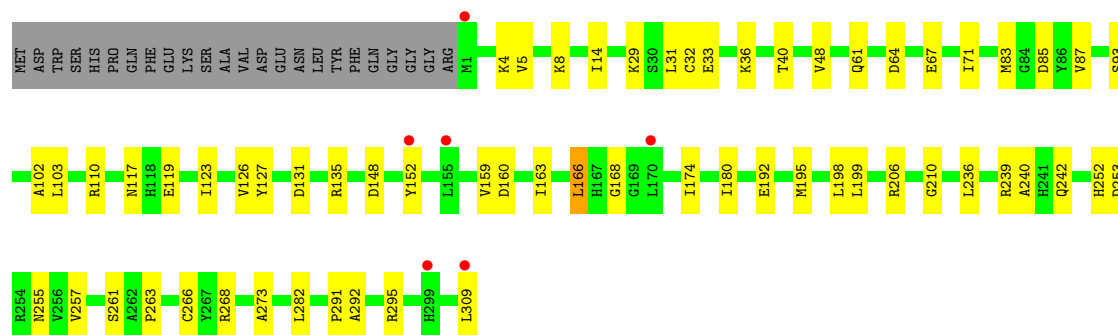


- Molecule 2: Serine/threonine-protein phosphatase 2A 56 kDa regulatory subunit epsilon isoform



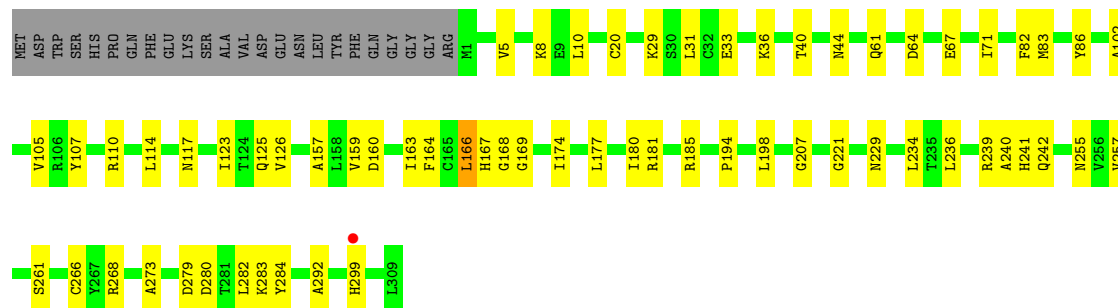
- Molecule 3: Serine/threonine-protein phosphatase 2A 65 kDa regulatory subunit A alpha isoform





- Molecule 3: Serine/threonine-protein phosphatase 2A 65 kDa regulatory subunit A alpha isoform

Chain F: 74% 19% 7%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	83.84Å 92.60Å 134.66Å 83.77° 72.46° 73.46°	Depositor
Resolution (Å)	128.36 – 3.15 128.36 – 3.15	Depositor EDS
% Data completeness (in resolution range)	96.4 (128.36-3.15) 96.4 (128.36-3.15)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.27 (at 3.13Å)	Xtrriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.221 , 0.263 0.219 , 0.261	Depositor DCC
R_{free} test set	3053 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	107.7	Xtrriage
Anisotropy	0.240	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 71.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.000 for -h,-k,-h+1	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	20861	wwPDB-VP
Average B, all atoms (Å ²)	117.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.81% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.24	0/4652	0.47	0/6315
1	D	0.23	0/4538	0.44	0/6158
2	B	0.24	0/3503	0.43	0/4737
2	E	0.25	0/3465	0.45	0/4685
3	C	0.24	0/2567	0.49	0/3479
3	F	0.24	0/2567	0.48	0/3479
All	All	0.24	0/21292	0.46	0/28853

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4578	0	4675	86	0
1	D	4466	0	4565	73	0
2	B	3420	0	3444	48	0
2	E	3383	0	3410	50	0
3	C	2505	0	2406	35	0
3	F	2505	0	2406	37	0
4	C	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	F	2	0	0	0	0
All	All	20861	0	20906	320	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (320) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:248:ILE:HG22	2:E:252:PHE:HE1	1.48	0.79
1:D:279:THR:HG22	1:D:283:LEU:HD12	1.71	0.73
1:A:206:ILE:HG13	1:A:243:LEU:HD13	1.70	0.71
1:D:334:VAL:HG21	1:D:368:LEU:HD12	1.72	0.71
1:D:90:LEU:HD12	1:D:131:LEU:HD13	1.72	0.70
1:D:136:ALA:HB1	1:D:173:LEU:HD21	1.72	0.69
1:A:28:ARG:NH1	1:A:61:ASP:OD2	2.28	0.66
1:A:206:ILE:HG21	1:A:243:LEU:HD22	1.77	0.66
1:A:352:LEU:HA	1:A:355:ILE:HD12	1.77	0.65
1:D:538:PHE:HB3	1:D:575:VAL:HG12	1.77	0.65
1:A:229:VAL:HG11	1:A:269:GLU:HG2	1.79	0.65
2:E:72:VAL:O	2:E:89:LYS:NZ	2.27	0.64
2:E:249:ILE:HA	2:E:252:PHE:CD1	2.33	0.64
1:D:93:LEU:HB3	1:D:112:LEU:HD11	1.78	0.63
2:B:256:LEU:HD12	2:B:295:ASP:HB2	1.80	0.63
1:D:183:ARG:HG3	1:D:220:VAL:HG12	1.80	0.63
1:D:322:ILE:HA	1:D:326:ILE:HB	1.81	0.62
2:B:376:ILE:HG23	2:B:383:ILE:HD11	1.81	0.62
1:A:136:ALA:HB1	1:A:173:LEU:HD21	1.81	0.62
1:D:87:HIS:HA	1:D:90:LEU:HD23	1.80	0.62
1:A:334:VAL:HG21	1:A:368:LEU:HD12	1.81	0.62
1:A:100:GLU:HA	1:A:142:THR:HG21	1.81	0.62
1:A:401:SER:HA	1:A:405:LEU:HB2	1.82	0.61
3:C:159:VAL:HB	3:C:163:ILE:HB	1.82	0.61
1:D:47:THR:HG23	1:D:51:LEU:HD23	1.82	0.61
1:D:199:ASP:HA	1:D:202:LYS:HE2	1.81	0.61
1:A:199:ASP:HA	1:A:202:LYS:HE2	1.83	0.60
1:D:401:SER:HA	1:D:405:LEU:HB2	1.83	0.60
2:E:256:LEU:HD12	2:E:295:ASP:HB2	1.83	0.60
1:A:47:THR:HG23	1:A:51:LEU:HD23	1.84	0.60
1:D:160:SER:O	1:D:163:LYS:NZ	2.32	0.60
2:B:269:ILE:HD11	2:B:302:VAL:HA	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:61:GLN:NE2	3:F:64:ASP:OD2	2.32	0.60
1:A:311:GLU:OE2	1:A:312:ASN:ND2	2.33	0.60
2:B:118:MET:O	2:B:122:ASN:ND2	2.26	0.60
2:E:118:MET:O	2:E:122:ASN:ND2	2.30	0.60
1:A:414:ASP:O	1:A:420:ARG:NH1	2.34	0.59
1:A:91:PRO:HB2	1:A:92:PRO:HD3	1.85	0.59
1:A:526:LEU:HD22	1:A:563:ILE:HG13	1.84	0.59
1:A:574:ASP:OD2	3:C:110:ARG:NH1	2.36	0.59
1:A:479:HIS:HA	1:A:483:ILE:HD12	1.85	0.58
1:D:414:ASP:O	1:D:420:ARG:NH1	2.34	0.58
1:D:479:HIS:HA	1:D:483:ILE:HD12	1.86	0.58
1:A:147:ALA:HA	1:A:150:LEU:HD23	1.85	0.58
1:A:229:VAL:HG21	1:A:266:LYS:HD3	1.86	0.58
1:A:11:TYR:O	1:A:46:ARG:NH2	2.36	0.58
1:A:228:CYS:SG	1:A:248:LEU:HD11	2.44	0.58
1:A:197:GLU:OE1	1:A:200:ASN:ND2	2.35	0.58
3:F:160:ASP:HB3	3:F:282:LEU:HD11	1.86	0.58
1:A:136:ALA:HB3	1:A:169:TYR:HE2	1.69	0.57
2:E:381:ASN:OD1	2:E:418:ASN:ND2	2.37	0.57
1:A:63:ASP:HB3	1:A:104:VAL:HG21	1.86	0.57
1:D:119:HIS:O	1:D:157:ARG:NH2	2.25	0.57
2:E:344:LEU:O	2:E:348:ILE:HD12	2.05	0.57
1:A:331:LYS:HD2	1:A:368:LEU:HD11	1.85	0.57
2:B:221:ILE:HG23	2:B:241:LEU:HD13	1.87	0.57
1:D:572:ASP:HB3	1:D:575:VAL:HG22	1.87	0.57
2:B:432:ASP:HA	2:B:435:ARG:HD2	1.86	0.57
2:E:353:SER:HA	2:E:394:ILE:HG13	1.87	0.57
3:C:61:GLN:NE2	3:C:64:ASP:OD2	2.36	0.57
2:E:401:PRO:HA	2:E:404:VAL:HG22	1.87	0.57
1:A:271:GLN:HG3	1:A:279:THR:HG21	1.87	0.57
1:A:538:PHE:HB3	1:A:575:VAL:HG12	1.86	0.56
1:A:381:ARG:O	1:A:385:ILE:HG13	2.05	0.56
2:E:404:VAL:HA	2:E:407:VAL:HG12	1.87	0.56
3:F:36:LYS:O	3:F:40:THR:OG1	2.22	0.56
1:A:535:ASN:HA	1:A:538:PHE:CE2	2.40	0.55
2:B:353:SER:HA	2:B:394:ILE:HG13	1.87	0.55
1:A:237:GLN:N	1:A:237:GLN:OE1	2.38	0.55
1:A:233:GLN:HG3	1:A:273:ALA:HB1	1.87	0.55
1:A:93:LEU:HB3	1:A:112:LEU:HD11	1.88	0.55
1:D:331:LYS:HD2	1:D:368:LEU:HD11	1.88	0.55
3:C:4:LYS:O	3:C:8:LYS:HG3	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:VAL:O	1:A:133:LYS:HG2	2.06	0.55
1:D:498:ARG:NH2	3:F:280:ASP:OD2	2.31	0.55
2:E:139:GLU:HB3	3:F:268:ARG:NH1	2.22	0.55
1:D:189:LEU:HD21	1:D:209:PHE:HB2	1.89	0.54
1:D:535:ASN:HA	1:D:538:PHE:CE2	2.41	0.54
2:E:376:ILE:HG23	2:E:383:ILE:HD11	1.88	0.54
3:C:5:VAL:HA	3:C:8:LYS:HD2	1.90	0.54
3:F:164:PHE:HB2	3:F:234:LEU:HD13	1.90	0.53
1:A:279:THR:HG22	1:A:283:LEU:HD12	1.89	0.53
1:A:322:ILE:HA	1:A:326:ILE:HB	1.90	0.53
2:B:74:PHE:HB3	2:B:86:LYS:HE2	1.90	0.53
3:C:123:ILE:HA	3:C:126:VAL:HG12	1.90	0.53
3:F:67:GLU:HB2	3:F:292:ALA:HB2	1.91	0.53
1:A:144:ARG:HB3	1:A:181:VAL:HG21	1.91	0.53
1:A:357:GLY:O	1:A:361:THR:HG23	2.08	0.53
1:A:572:ASP:HB3	1:A:575:VAL:HG22	1.91	0.52
1:D:303:SER:HB3	1:D:345:LEU:HB2	1.90	0.52
1:D:526:LEU:HD22	1:D:563:ILE:HG13	1.90	0.52
1:D:271:GLN:HG3	1:D:279:THR:HG21	1.92	0.52
1:A:544:LEU:HD22	1:A:560:VAL:HG13	1.92	0.52
2:E:120:SER:O	2:E:124:PHE:HB2	2.09	0.52
1:A:112:LEU:HB3	1:A:150:LEU:HD11	1.92	0.52
2:B:292:LEU:HD21	2:B:302:VAL:HG21	1.90	0.52
2:E:107:LEU:HB2	2:E:166:GLU:HG3	1.92	0.52
3:C:29:LYS:NZ	3:C:33:GLU:OE2	2.43	0.52
1:A:509:SER:HA	1:A:517:THR:HG21	1.92	0.51
2:E:292:LEU:HD21	2:E:302:VAL:HG21	1.91	0.51
3:F:207:GLY:HA2	3:F:221:GLY:HA3	1.92	0.51
1:D:317:CYS:O	1:D:321:VAL:HG23	2.10	0.51
3:C:83:MET:HE3	3:C:240:ALA:HB2	1.92	0.51
1:D:381:ARG:O	1:D:385:ILE:HG13	2.10	0.51
3:C:67:GLU:HB2	3:C:292:ALA:HB2	1.93	0.51
2:B:430:LYS:HA	2:B:433:ARG:HB2	1.92	0.51
1:D:357:GLY:O	1:D:361:THR:HG23	2.11	0.51
2:E:93:LEU:HD13	2:E:153:LEU:HB2	1.93	0.51
1:A:240:LEU:HD13	1:A:274:VAL:HG13	1.92	0.50
3:F:123:ILE:HA	3:F:126:VAL:HG12	1.93	0.50
2:B:401:PRO:HA	2:B:404:VAL:HG22	1.93	0.50
1:D:537:ARG:NE	1:D:570:ASP:OD2	2.43	0.50
2:E:156:GLU:HA	2:E:159:ILE:HG22	1.94	0.50
3:C:31:LEU:HD11	3:C:102:ALA:HA	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:544:LEU:HD22	1:D:560:VAL:HG13	1.94	0.50
1:D:23:GLU:HB3	1:D:27:LEU:HD12	1.94	0.49
2:E:390:SER:O	2:E:394:ILE:HG12	2.12	0.49
2:B:254:LEU:HB3	2:B:255:PRO:HD3	1.95	0.49
1:A:398:ARG:O	1:A:402:GLN:HG2	2.13	0.49
1:A:424:ILE:HG12	1:A:450:TRP:CE3	2.48	0.49
2:B:178:GLN:HB3	2:B:216:PHE:CE2	2.48	0.49
2:B:107:LEU:HB2	2:B:166:GLU:HG3	1.95	0.49
1:D:55:LEU:HD13	1:D:69:LEU:HD11	1.95	0.49
2:E:254:LEU:HB3	2:E:255:PRO:HD3	1.93	0.49
1:A:317:CYS:O	1:A:321:VAL:HG23	2.12	0.49
3:C:166:LEU:O	3:C:239:ARG:HA	2.13	0.49
2:E:356:HIS:NE2	3:F:125:GLN:O	2.40	0.49
1:A:35:LEU:HG	1:A:38:ILE:HD11	1.95	0.48
1:D:197:GLU:OE1	1:D:200:ASN:ND2	2.41	0.48
2:E:249:ILE:HA	2:E:252:PHE:CE1	2.49	0.48
3:C:131:ASP:O	3:C:135:ARG:HG3	2.13	0.48
2:E:45:LEU:N	2:E:85:MET:SD	2.86	0.48
2:B:181:VAL:HG21	2:B:217:ILE:HD12	1.96	0.48
2:B:367:TRP:CD1	2:B:410:VAL:HG13	2.49	0.47
2:E:65:LYS:O	2:E:69:GLN:HG3	2.13	0.47
3:F:159:VAL:HB	3:F:163:ILE:HB	1.95	0.47
3:F:114:LEU:HD11	3:F:157:ALA:HB2	1.95	0.47
1:A:14:ALA:HA	1:A:17:ILE:HG12	1.97	0.47
1:D:100:GLU:HA	1:D:142:THR:HG21	1.96	0.47
1:D:408:ILE:HG23	1:D:423:ILE:HD12	1.95	0.47
1:A:427:MET:HG3	1:A:450:TRP:HZ3	1.79	0.47
1:A:307:LYS:HA	1:A:352:LEU:HD21	1.96	0.47
1:D:218:ASP:OD1	1:D:218:ASP:N	2.48	0.47
3:C:87:VAL:HG12	3:C:93:SER:HB3	1.97	0.47
1:D:70:ALA:HB2	1:D:96:LEU:HD13	1.96	0.47
1:D:279:THR:HA	1:D:283:LEU:HB2	1.96	0.47
1:A:276:PRO:O	1:A:279:THR:OG1	2.30	0.47
2:B:381:ASN:OD1	2:B:418:ASN:ND2	2.35	0.46
2:B:390:SER:O	2:B:394:ILE:HG12	2.15	0.46
2:E:252:PHE:CE2	2:E:260:HIS:CG	3.03	0.46
1:D:144:ARG:HB3	1:D:173:LEU:HD11	1.96	0.46
2:E:248:ILE:O	2:E:252:PHE:HD1	1.98	0.46
2:B:82:ASP:O	2:B:86:LYS:HG3	2.14	0.46
3:C:67:GLU:O	3:C:71:ILE:HG12	2.15	0.46
1:D:278:ILE:HD12	1:D:278:ILE:H	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:5:VAL:HA	3:F:8:LYS:HD2	1.98	0.46
1:D:179:PRO:HD2	1:D:180:MET:HE1	1.98	0.46
1:D:239:ASP:HB3	1:D:243:LEU:HD12	1.98	0.46
1:A:163:LYS:HE2	1:A:167:ARG:HH22	1.80	0.46
2:B:344:LEU:O	2:B:348:ILE:HD12	2.15	0.46
3:C:14:ILE:HD13	3:C:103:LEU:HD23	1.96	0.46
1:D:424:ILE:HG12	1:D:450:TRP:CE3	2.51	0.46
3:F:236:LEU:HD11	3:F:257:VAL:HG12	1.98	0.46
3:F:107:TYR:HB3	3:F:110:ARG:HB2	1.97	0.46
1:A:378:PRO:HB3	1:A:416:LYS:HG3	1.97	0.45
1:A:408:ILE:HG23	1:A:423:ILE:HD12	1.97	0.45
1:D:455:VAL:HG13	3:F:71:ILE:HD13	1.98	0.45
3:F:44:ASN:OD1	3:F:185:ARG:NH1	2.46	0.45
1:D:352:LEU:HA	1:D:355:ILE:HD12	1.98	0.45
1:A:222:LEU:HG	1:A:223:LEU:HD12	1.97	0.45
2:B:261:LYS:HG2	2:B:298:LEU:HD21	1.99	0.45
1:A:222:LEU:HA	1:A:259:VAL:HG23	1.99	0.45
2:B:120:SER:O	2:B:124:PHE:HB2	2.17	0.45
1:D:23:GLU:O	1:D:28:ARG:NH2	2.44	0.45
2:E:221:ILE:HG21	2:E:245:LEU:HD11	1.97	0.45
2:E:256:LEU:HD23	2:E:256:LEU:HA	1.83	0.45
2:E:422:PHE:O	2:E:426:THR:HG22	2.16	0.45
3:F:169:GLY:O	3:F:198:LEU:HA	2.17	0.45
1:D:378:PRO:HB3	1:D:416:LYS:HG3	1.98	0.45
3:C:206:ARG:HH21	3:C:210:GLY:HA3	1.81	0.45
2:E:64:LEU:HD21	2:E:111:THR:HG22	1.99	0.45
2:E:284:LEU:O	2:E:288:ILE:HG12	2.17	0.44
1:A:90:LEU:HD21	1:A:128:PHE:HD1	1.83	0.44
3:C:4:LYS:H	3:C:4:LYS:HD2	1.83	0.44
3:C:180:ILE:HG12	3:C:198:LEU:HD11	1.98	0.44
2:E:63:PHE:CE1	2:E:96:LEU:HD22	2.52	0.44
1:A:424:ILE:HD11	1:A:458:ILE:HG23	1.99	0.44
1:A:441:GLU:HG2	1:A:442:LYS:HG2	1.99	0.44
1:D:24:ASP:O	1:D:28:ARG:HG3	2.18	0.44
3:C:160:ASP:HB3	3:C:282:LEU:HD11	1.99	0.44
3:C:261:SER:HA	3:C:273:ALA:HB1	1.98	0.44
1:D:219:SER:O	1:D:223:LEU:HD12	2.16	0.44
1:A:303:SER:HA	1:A:306:VAL:HG23	1.98	0.44
1:A:314:SER:HB3	1:A:317:CYS:SG	2.58	0.44
1:D:209:PHE:HE2	1:D:247:THR:HG1	1.65	0.44
2:E:138:GLU:HG3	2:E:139:GLU:HG2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:90:LEU:HD21	1:D:119:HIS:NE2	2.32	0.44
1:A:81:GLY:HA3	1:A:85:TYR:HD2	1.82	0.44
2:B:221:ILE:HG21	2:B:245:LEU:HD11	1.99	0.44
1:A:537:ARG:NE	1:A:570:ASP:OD2	2.51	0.44
3:C:266:CYS:O	3:C:268:ARG:HG3	2.18	0.44
2:E:94:ASN:HA	2:E:97:VAL:HG22	2.00	0.44
2:B:438:LYS:HE2	2:B:438:LYS:HB3	1.85	0.44
1:D:91:PRO:HB2	1:D:92:PRO:HD3	1.99	0.44
1:D:101:GLU:HG3	1:D:103:VAL:HG22	1.99	0.44
2:B:243:GLU:HG3	2:B:283:GLN:HG2	2.00	0.43
1:D:377:CYS:HB3	1:D:380:VAL:HG12	2.00	0.43
1:A:268:THR:HG21	1:A:308:GLU:HG2	2.00	0.43
1:A:364:HIS:O	1:A:368:LEU:HD23	2.17	0.43
2:B:304:ARG:NH1	2:B:343:PRO:HG3	2.33	0.43
2:E:205:ARG:HD3	2:E:205:ARG:HA	1.78	0.43
3:F:83:MET:HE3	3:F:240:ALA:HB2	2.00	0.43
1:A:272:LYS:HD2	1:A:272:LYS:HA	1.76	0.43
2:B:433:ARG:HA	2:B:436:GLU:HG2	2.01	0.43
2:E:62:LEU:HD21	2:E:66:LYS:HE2	1.99	0.43
1:D:295:GLU:O	1:D:299:ARG:HG3	2.18	0.43
1:A:136:ALA:HB3	1:A:169:TYR:CE2	2.52	0.43
2:B:119:VAL:O	2:B:123:ILE:HG12	2.18	0.43
3:C:236:LEU:HD11	3:C:257:VAL:HG12	2.00	0.43
1:A:368:LEU:O	1:A:372:GLN:HG3	2.18	0.43
2:B:91:SER:O	2:B:95:GLU:HG3	2.19	0.43
2:B:93:LEU:HD13	2:B:153:LEU:HB2	2.00	0.43
3:C:36:LYS:HD3	3:C:152:TYR:CE1	2.53	0.43
3:C:240:ALA:O	3:C:242:GLN:N	2.50	0.43
1:D:284:VAL:HB	1:D:285:PRO:HD3	2.01	0.43
1:D:318:ARG:O	1:D:322:ILE:HD12	2.19	0.43
2:E:64:LEU:O	2:E:68:GLN:HG3	2.19	0.43
2:E:243:GLU:HG3	2:E:283:GLN:HG2	2.00	0.43
2:E:319:VAL:HG13	2:E:362:ARG:HG2	1.99	0.43
3:F:31:LEU:HD11	3:F:102:ALA:HA	2.00	0.43
3:F:194:PRO:O	3:F:198:LEU:HG	2.19	0.43
2:B:162:LEU:HD21	2:B:206:ILE:HG13	2.00	0.43
2:E:288:ILE:O	2:E:292:LEU:HG	2.19	0.43
3:F:10:LEU:HD11	3:F:105:VAL:HG12	2.00	0.43
2:B:54:VAL:HG21	2:B:62:LEU:HD23	2.01	0.43
2:B:324:GLU:O	2:B:328:ILE:HD12	2.18	0.43
2:B:64:LEU:O	2:B:68:GLN:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:171:ARG:NH1	1:D:172:ASN:OD1	2.53	0.42
2:E:248:ILE:HG22	2:E:252:PHE:CE1	2.39	0.42
3:F:174:ILE:HD12	3:F:180:ILE:HG13	2.01	0.42
3:F:261:SER:HA	3:F:273:ALA:HB1	2.01	0.42
1:A:455:VAL:HG13	3:C:71:ILE:HA	2.01	0.42
2:B:372:ILE:O	2:B:376:ILE:HG13	2.19	0.42
1:A:101:GLU:O	1:A:105:ARG:HG2	2.19	0.42
1:D:152:SER:OG	1:D:191:GLU:OE2	2.25	0.42
2:E:139:GLU:HB3	3:F:268:ARG:HH12	1.84	0.42
1:A:30:ASN:HD22	1:A:30:ASN:HA	1.64	0.42
3:F:29:LYS:NZ	3:F:33:GLU:OE2	2.52	0.42
3:C:32:CYS:O	3:C:36:LYS:HG3	2.20	0.42
3:F:177:LEU:O	3:F:181:ARG:HG3	2.20	0.42
1:A:245:MET:N	1:A:246:PRO:HD2	2.34	0.42
1:A:334:VAL:HG21	1:A:368:LEU:CD1	2.47	0.42
2:B:404:VAL:HA	2:B:407:VAL:HG12	2.02	0.42
3:F:266:CYS:O	3:F:268:ARG:HG3	2.19	0.42
3:F:268:ARG:HE	3:F:268:ARG:HB2	1.67	0.42
1:D:227:ALA:O	1:D:231:ILE:HG13	2.20	0.42
2:B:295:ASP:HB3	2:B:298:LEU:HD12	2.00	0.42
1:D:254:ASP:OD1	1:D:255:LYS:N	2.52	0.42
3:F:82:PHE:HB3	3:F:86:TYR:HE1	1.85	0.42
1:A:54:PHE:O	1:A:58:THR:HG22	2.20	0.42
2:B:312:LYS:HG2	3:C:309:LEU:HB3	2.02	0.42
2:E:269:ILE:HD11	2:E:302:VAL:HA	2.01	0.42
3:F:240:ALA:O	3:F:242:GLN:N	2.52	0.42
1:D:38:ILE:O	1:D:42:LEU:HG	2.20	0.41
1:D:63:ASP:HB3	1:D:104:VAL:HG21	2.02	0.41
3:F:117:ASN:H	3:F:167:HIS:CD2	2.37	0.41
3:F:279:ASP:HB2	3:F:283:LYS:HB2	2.02	0.41
1:A:362:ILE:HA	1:A:366:LEU:HG	2.02	0.41
3:C:48:VAL:O	3:C:159:VAL:HA	2.20	0.41
1:D:398:ARG:O	1:D:402:GLN:HG2	2.21	0.41
2:B:422:PHE:O	2:B:426:THR:HG22	2.20	0.41
1:D:197:GLU:O	1:D:201:VAL:HG13	2.20	0.41
1:D:249:ARG:O	1:D:253:GLU:HG2	2.20	0.41
1:A:7:ASP:OD1	1:A:7:ASP:N	2.54	0.41
1:A:565:GLU:O	1:A:568:THR:OG1	2.39	0.41
2:B:155:TYR:HB3	2:B:198:TYR:CD1	2.56	0.41
1:D:147:ALA:HA	1:D:150:LEU:HD23	2.02	0.41
1:D:201:VAL:O	1:D:206:ILE:HG12	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:48:LEU:HD11	2:B:65:LYS:HD2	2.02	0.41
2:B:391:LEU:HD23	2:B:407:VAL:HG23	2.02	0.41
2:E:217:ILE:O	2:E:221:ILE:HG13	2.21	0.41
1:A:179:PRO:HA	1:A:182:ARG:HB2	2.03	0.41
3:C:123:ILE:HG23	3:C:127:TYR:HD2	1.86	0.41
1:D:279:THR:O	1:D:284:VAL:HG23	2.21	0.41
2:E:66:LYS:HD3	2:E:92:THR:HG23	2.03	0.41
1:A:62:GLU:HG3	1:A:64:GLU:H	1.86	0.41
2:B:284:LEU:O	2:B:288:ILE:HG12	2.20	0.41
3:F:229:ASN:ND2	3:F:255:ASN:OD1	2.52	0.41
1:A:105:ARG:HB2	1:A:146:SER:OG	2.21	0.41
2:B:217:ILE:O	2:B:221:ILE:HG13	2.20	0.41
2:B:373:MET:O	2:B:377:GLU:HG2	2.21	0.41
2:B:402:ALA:O	2:B:406:LEU:HD23	2.20	0.41
3:C:263:PRO:HB2	3:C:291:PRO:HD3	2.03	0.41
1:D:35:LEU:HD21	1:D:55:LEU:HD11	2.02	0.41
2:E:119:VAL:O	2:E:123:ILE:HG12	2.21	0.41
2:E:322:LEU:HD12	2:E:362:ARG:HB3	2.03	0.41
2:E:431:SER:O	2:E:435:ARG:HG3	2.21	0.41
1:A:354:PRO:HD3	1:A:390:CYS:SG	2.61	0.41
3:F:239:ARG:NH2	3:F:241:HIS:HB3	2.36	0.41
1:A:451:LEU:HD11	1:A:466:LEU:HD11	2.03	0.40
2:E:391:LEU:HD23	2:E:407:VAL:HG23	2.03	0.40
1:A:140:TRP:CZ2	2:B:266:LYS:HB3	2.56	0.40
1:A:286:ALA:O	1:A:290:LEU:HG	2.21	0.40
1:D:377:CYS:HA	1:D:378:PRO:HD3	1.97	0.40
2:E:292:LEU:HD22	2:E:299:THR:HG22	2.03	0.40
3:F:166:LEU:O	3:F:239:ARG:HA	2.21	0.40
1:A:237:GLN:HA	1:A:240:LEU:HD12	2.03	0.40
2:B:362:ARG:HA	2:B:362:ARG:HD2	1.84	0.40
3:C:117:ASN:HB3	3:C:199:LEU:O	2.21	0.40
3:C:252:HIS:O	3:C:255:ASN:HB2	2.22	0.40
2:E:295:ASP:HB3	2:E:298:LEU:HD12	2.03	0.40
1:A:89:LEU:O	1:A:93:LEU:HD23	2.21	0.40
1:A:420:ARG:O	1:A:424:ILE:HG13	2.21	0.40
3:C:36:LYS:O	3:C:40:THR:OG1	2.31	0.40
3:C:85:ASP:N	3:C:119:GLU:OE2	2.54	0.40
1:D:73:LEU:HB3	1:D:93:LEU:HD21	2.04	0.40
1:D:173:LEU:HD12	1:D:181:VAL:HG21	2.03	0.40
3:C:174:ILE:HD12	3:C:180:ILE:HG13	2.03	0.40
1:D:388:LEU:HD23	1:D:388:LEU:HA	1.97	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:8:LYS:H	3:F:8:LYS:HG3	1.66	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	587/612 (96%)	563 (96%)	22 (4%)	2 (0%)	41	73
1	D	571/612 (93%)	549 (96%)	21 (4%)	1 (0%)	47	78
2	B	409/467 (88%)	386 (94%)	22 (5%)	1 (0%)	47	78
2	E	405/467 (87%)	379 (94%)	26 (6%)	0	100	100
3	C	307/333 (92%)	287 (94%)	19 (6%)	1 (0%)	41	73
3	F	307/333 (92%)	285 (93%)	20 (6%)	2 (1%)	22	59
All	All	2586/2824 (92%)	2449 (95%)	130 (5%)	7 (0%)	41	73

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	F	299	HIS
1	A	36	SER
1	D	36	SER
1	A	276	PRO
2	B	47	PRO
3	F	168	GLY
3	C	168	GLY

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	512/531 (96%)	504 (98%)	8 (2%)	62	83
1	D	501/531 (94%)	496 (99%)	5 (1%)	76	89
2	B	388/438 (89%)	380 (98%)	8 (2%)	53	78
2	E	383/438 (87%)	373 (97%)	10 (3%)	46	74
3	C	274/294 (93%)	268 (98%)	6 (2%)	52	77
3	F	274/294 (93%)	271 (99%)	3 (1%)	73	88
All	All	2332/2526 (92%)	2292 (98%)	40 (2%)	60	82

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	GLN
1	A	54	PHE
1	A	60	TYR
1	A	139	ASP
1	A	180	MET
1	A	241	GLU
1	A	308	GLU
1	A	324	SER
2	B	160	ARG
2	B	194	ARG
2	B	205	ARG
2	B	218	ARG
2	B	291	PHE
2	B	422	PHE
2	B	431	SER
2	B	443	ARG
3	C	148	ASP
3	C	166	LEU
3	C	192	GLU
3	C	195	MET
3	C	253	ASP
3	C	295	ARG

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Mol	Chain	Res	Type
1	D	180	MET
1	D	223	LEU
1	D	238	GLU
1	D	239	ASP
1	D	324	SER
2	E	118	MET
2	E	160	ARG
2	E	194	ARG
2	E	205	ARG
2	E	257	LYS
2	E	374	SER
2	E	392	TYR
2	E	421	MET
2	E	422	PHE
2	E	443	ARG
3	F	20	CYS
3	F	166	LEU
3	F	284	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	589/612 (96%)	0.35	41 (6%) 16 8	70, 126, 174, 199	0
1	D	573/612 (93%)	0.13	3 (0%) 91 86	66, 100, 150, 183	0
2	B	410/467 (87%)	0.19	19 (4%) 32 18	95, 138, 180, 210	0
2	E	407/467 (87%)	0.15	8 (1%) 65 50	71, 118, 174, 201	0
3	C	309/333 (92%)	0.04	6 (1%) 66 53	68, 100, 137, 196	0
3	F	309/333 (92%)	-0.00	1 (0%) 94 92	66, 92, 128, 194	0
All	All	2597/2824 (91%)	0.17	78 (3%) 50 33	66, 111, 171, 210	0

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	128	PHE	6.1
1	A	124	LEU	5.1
1	A	89	LEU	5.0
2	B	302	VAL	4.9
1	A	151	PHE	4.8
1	A	93	LEU	4.7
1	A	51	LEU	4.7
1	A	150	LEU	4.0
1	A	589	ALA	3.9
3	C	309	LEU	3.8
1	A	88	CYS	3.8
2	E	256	LEU	3.8
2	B	376	ILE	3.7
2	B	138	GLU	3.6
1	A	235	LEU	3.5
1	A	166	LEU	3.4
1	A	209	PHE	3.4
3	F	299	HIS	3.2
2	E	137	PRO	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	274	VAL	3.2
1	A	231	ILE	3.1
1	A	38	ILE	3.1
1	A	16	LEU	3.1
1	A	147	ALA	3.0
2	B	261	LYS	3.0
1	A	152	SER	2.9
1	A	11	TYR	2.9
1	A	201	VAL	2.9
1	A	37	THR	2.8
2	E	49	PRO	2.8
1	A	55	LEU	2.7
1	A	196	LEU	2.7
1	A	239	ASP	2.7
3	C	1	MET	2.7
3	C	155	LEU	2.6
2	E	99	TYR	2.6
2	B	102	ILE	2.6
1	A	154	CYS	2.6
1	A	356	LEU	2.5
1	A	244	VAL	2.5
1	A	34	LYS	2.5
1	A	73	LEU	2.4
1	A	283	LEU	2.4
1	D	589	ALA	2.4
1	A	17	ILE	2.4
2	B	167	PHE	2.4
3	C	299	HIS	2.3
1	A	12	PRO	2.3
2	B	306	LEU	2.3
2	B	211	LEU	2.3
2	B	394	ILE	2.3
1	A	69	LEU	2.3
2	B	100	ILE	2.3
3	C	152	TYR	2.2
1	A	21	ARG	2.2
1	D	430	LEU	2.2
1	D	20	LEU	2.2
2	E	100	ILE	2.2
1	A	385	ILE	2.2
1	A	45	GLU	2.2
2	E	184	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	248	LEU	2.1
2	B	388	PHE	2.1
2	B	93	LEU	2.1
2	E	119	VAL	2.1
2	B	348	ILE	2.1
1	A	240	LEU	2.1
2	B	170	SER	2.1
1	A	77	THR	2.1
2	B	341	GLN	2.1
3	C	170	LEU	2.1
2	E	388	PHE	2.1
1	A	345	LEU	2.1
2	B	74	PHE	2.1
2	B	169	PRO	2.1
2	B	378	GLU	2.1
1	A	224	ALA	2.1
2	B	383	ILE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	MN	F	402	1/1	0.80	0.30	152,152,152,152	0
4	MN	F	401	1/1	0.92	0.29	83,83,83,83	0
4	MN	C	402	1/1	0.96	0.24	149,149,149,149	0
4	MN	C	401	1/1	0.97	0.28	83,83,83,83	0

6.5 Other polymers [i](#)

There are no such residues in this entry.